

Mathematical Problems in Quantum
Mechanics

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**CURVED QUANTUM
WAVEGUIDES WITH
COMBINED BOUNDARY
CONDITIONS**

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J. Dittrich, J K, J. Phys. A **35** (2002), L269–275.

D. Krejčířík, J K, math-ph/0306008.

Program

1. Introduction (What are QW?; Various boundary conditions)
2. Preliminaries (Configuration space; Hamiltonian)
3. Energy spectrum (Essential spectrum; Existence (absence) of discrete spectrum)
4. Conclusions (Comparison with known results; Open problems)

1. Introduction

What are quantum waveguides?

Semiconductor or metallic microstructures of the tube like shape.

- (a) small size $10 - 100 \text{ nm}$;
- (b) high purity (e^- mean free path $\sim \mu\text{m}$);
- (c) crystallic structure.

Physical background:

1. J. T. Londergan, J. P. Carini, and D. P. Murdock, *Binding and scattering in 2-dimensional systems*, LNP, vol. m60, Springer, Berlin, 1999.
2. S. Datta, *Electronic transport in mesoscopic systems*, Camb.Univ.Press, Cambridge, 1995.
3. P. Duclos and P. Exner, *Curvature-induced bound states in quantum waveguides in 2 and 3 dimensions*, Rev.Math.Phys. **7** (1995), 73–102.

Our model

free particle of an effective mass m^* living in nontrivial spatial region Ω
impenetrable walls: suitable b.c.

1. *Dirichlet b.c.* (semiconductor structures)
2. *Neumann b.c.* (metallic structures, acoustic or electromagnetic waveguides)
3. Waveguides with *combined* Dirichlet and Neumann b.c. on different parts of boundary

(more realistic models allow for quantum tunneling)

Mathematical point of view: spectrum of $-\Delta$ ($\hbar^2/(2m^*) = 1$) acting in the Hilbert space $L^2(\Omega)$

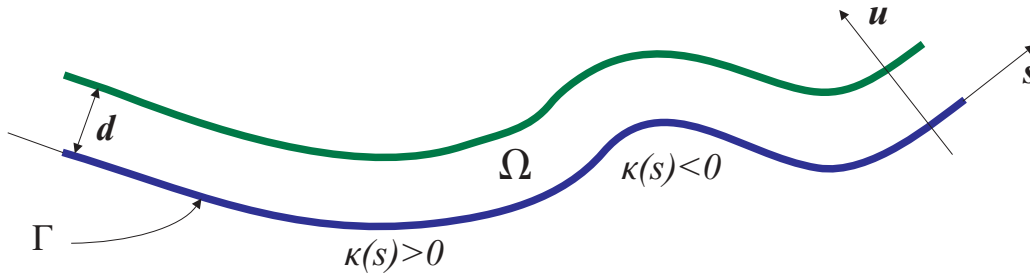
2. Preliminaries

Configuration space

- ◇ $\Gamma : \mathbb{R} \rightarrow \mathbb{R}^2$... C^2 infinite plane curve
- ◇ $\nu := (-\dot{\Gamma}^2, \dot{\Gamma}^1)$... unit normal vector field
- ◇ $\kappa := \det(\dot{\Gamma}, \ddot{\Gamma})$... signed curvature
- ◇ $\Omega_0 := \mathbb{R} \times (0, d)$... straight strip of width d
- ◇ $\mathcal{L} : \mathbb{R}^2 \rightarrow \mathbb{R}^2 : \{(s, u) \mapsto \Gamma(s) + u\nu(s)\}$
- ◇ $\Omega := \mathcal{L}(\Omega_0)$... curved strip along Γ
- ◇ $\kappa_{\pm} := \max\{0, \pm\kappa\}$
- ◇ $\alpha := \int_{\mathbb{R}} \kappa(s) ds$... bending angle

- Assumptions : $\diamond \Omega$ is not self – intersecting
 $\diamond \kappa \in L^\infty(\mathbb{R}), d\|\kappa_+\|_{L^\infty(\mathbb{R})} < 1$

$\mathcal{L} : \Omega_0 \rightarrow \Omega \dots C^1$ -diffeomorphism;
 \mathcal{L}^{-1} defines natural coordinates (s, u)



— ... Dirichlet b.c. — ... Neumann b.c.

Hilbert space: $L^2(\Omega) \rightarrow L^2(\Omega_0, (1 - u\kappa(s)) du ds)$

Hamiltonian

unique s.-a. operator, whose quadratic form is

$$Q(\psi, \varphi) := \int_{\Omega_0} \left(\frac{\overline{\partial\psi} \partial\varphi}{\partial s \partial s} + \frac{\overline{\partial\psi} \partial\varphi}{\partial u \partial u} (1 - u\kappa) \right) du ds$$

$$\text{Dom } Q := \{ \psi \in W^{1,2}(\Omega_0) \mid \psi(s, 0) = 0 \}$$

associated operator: H

$\Gamma \in C^3(\mathbb{R}) \implies$ Laplace–Beltrami operator

$$-\frac{1}{(1-u\kappa)^2} \partial_{ss}^2 - \frac{u\kappa}{(1-u\kappa)^3} \partial_s - \partial_{uu}^2 + \frac{\kappa}{1-u\kappa} \partial_u$$

operator domain $\text{Dom } H$

$$\left\{ \psi \in W^{2,2}(\Omega_0) \mid \psi(s, 0) = 0, \partial_u \psi(s, d) = 0 \right\}$$

3. Energy spectrum

Essential spectrum

Theorem:

$$\lim_{|s| \rightarrow \infty} \kappa(s) = 0 \implies \sigma_{\text{ess}}(H) = \left[\frac{\pi^2}{4d^2}, \infty \right)$$

PROOF: 1. D-N Bracketing.

2. Generalized Weyl criterion. □

Y. Dermenjian, M. Durand, and V. Iftimie, Commun. in Partial Differential Equations **23** (1998), no. 1&2, 141–169.

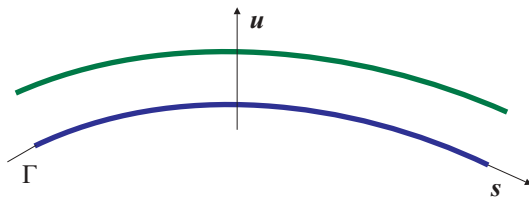
Discrete spectrum

Theorem:

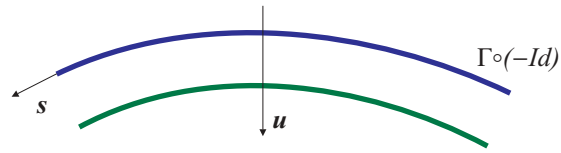
(i) Assume $\kappa \neq 0$. If one of
 (a) $\kappa \in L^1(\mathbb{R})$ and $\alpha \leq 0$
 (b) $\kappa_- \neq 0$ and d is small enough
 is satisfied then $\inf \sigma(H) < \frac{\pi^2}{4d^2}$.

(ii) If $\kappa_- \equiv 0$ then $\inf \sigma(H) \geq \frac{\pi^2}{4d^2}$.

$\alpha < 0$



$\alpha > 0$



PROOF: Existence - variationally.

Absence - $\forall \psi \in \text{Dom } Q_{DN}^\kappa$:

$$Q_{DN}^\kappa[\psi] - \frac{\pi^2}{4d^2} \|\psi\|_{L^2(\Omega_0, d\Omega)}^2 \geq 0. \quad \square$$

Corollary: Assume $\lim_{|s| \rightarrow \infty} \kappa(s) = 0$. Then

(i) $\implies H$ has an isolated eigenvalue;

(ii) $\implies \sigma_{\text{disc}}(H) = \emptyset$.

Some properties of discrete eigenvalues

Proposition: Assume $\kappa \neq 0$, $\text{supp } \kappa \subset [-s_0, s_0]$, $\alpha \leq 0$. Then $\inf \sigma(H) \leq \frac{\pi^2}{4d^2} - C \left(\frac{\alpha}{\pi}\right)^2$.

Remarks:

1. Dirichlet b.c. $\implies \inf \sigma(H) \leq \frac{\pi^2}{d^2} - \tilde{C} \left(\frac{\alpha}{\pi}\right)^4$

2. mildly curved strips Dirichlet strips: $\{\Gamma_\beta\}_{\beta>0}$

$$\kappa_\beta := \beta\kappa \implies \alpha_\beta = \beta\alpha$$

$$\inf \sigma(H) = \frac{\pi^2}{d^2} - \tilde{C}\beta^4 + \mathcal{O}(\beta^5).$$

3. thin strips

Combined: $\frac{\pi^2}{4d^2} - \inf \sigma(H) \geq -\frac{\alpha}{2ds_0} + \mathcal{O}(d^{-1/2})$

Dirichlet: $\frac{\pi^2}{d^2} - \inf \sigma(H) \geq \tilde{C}_0 \left(\frac{\alpha}{\pi}\right)^4 + \mathcal{O}(d)$

Exact asymptotic $\frac{\pi^2}{d^2} - \inf \sigma(H) = -\lambda + \mathcal{O}(d)$,

$\lambda \dots$ 1.eigenvalue $-d^2/(ds^2) - \kappa^2/4$

4. Conclusions

Comparison with known results

Assume only asymptotically straight strips.

Dirichlet b.c.: $\kappa \neq 0 \implies \sigma_{\text{disc}}(H) \neq \emptyset$.

P. Exner and P. Šeba, J.Math.Phys.**30** (1989), 2574–2580.

J. Goldstone and R. L. Jaffe, Phys.Rev.B **45** (1992), 14100–14107.

Neumann b.c.: $\sigma_{\text{disc}}(H) = \emptyset$.

Combined b.c.: existence of σ_{disc} depends on κ .

Open problems

more complicated combination of b.c.

higher dimensions

b.c. $a\psi + b\partial_\nu\psi = 0$

nature of essential spectrum